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Title: Advanced Research Capabilities for Neutron Scattering

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Los Alamos
NATIONAL LABORATORY

Advanced Research Capabilities for Neutron Scattering

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Abstract

This project covered a range of new technologies that can potentially improve the performance of neutron spectrometers at LANSCE and elsewhere. The project was broken down into four sections: Novel Position-Sensitive Neutron Detectors; Beam Optics and Choppers for Neutron Scattering Applications; Development of Monte-Carlo Simulation Tools for Neutron Instrument Design; and Development of Time-Resolved Cold-Neutron Radiography Methods.

A. Novel Position-Sensitive Detectors

Background and Research Objectives

Many of the projects envisaged for supporting the Stockpile Stewardship Program at LANSCE require neutron detectors. Currently nearly all of these are limited to what is available commercially. With this project we intend to broaden the range of options available for neutron detectors at Los Alamos Neutron Scattering Center by leveraging expertise and infrastructure available from the nuclear and particle physics programs at LANL. The goal of this work is to develop new detector technologies using existing expertise and infrastructure from the nuclear and particle physics programs at LANL.

Importance to LANL's Science and Technology Base and National R&D Needs

LANSCE provides many new capabilities for Stockpile Stewardship Program. Currently the facility and many of the instruments are undergoing a major upgrade. Our overall goal is to improve the detector technology available in the future at LANSCE.

Scientific Approach and Accomplishments

Detectors for High Energy Neutron Radiography

One objective emphasizes an imaging detector for high-energy neutrons for neutron radiography. High-energy neutrons are much better matched to radiography of thick weapon components than X-rays because of the longer mean free paths.

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Because of this, a given incident flux provides more accurate radiographic information and smaller scatter background.

Additionally, the larger cross-sections for neutrons on light isotopes lead to more contrast from low-A materials shielded by heavier isotopes in composite objects.

One difficulty with using medium energy neutrons as a radiographic probe is the absence of any suitable imaging detectors. In our initial work we have shown that good position resolution can be obtained using a high-density converter coupled to a position sensitive detector. Charged particles produced by neutron interactions in the converter are imaged in the detector. Because of the high rates involved, tracking is not possible, so it is important to minimize the thickness of the package to limit the blurring introduced by propagating the charge particles. Initial work concentrated on building one layer of an active readout imaging ion chamber [1]. This detector obtained about 1% detector quantum efficiency and about one millimeter position resolution.

We performed experiments at the Weapons Nuclear Research Facility (WNR) to demonstrate a new technology using stacked image plates and 1.5 millimeter thick copper converters. The ion chamber was replaced with an image plate. An image of a drill motor in its case is shown in figure 1. A special target was developed for the WNR to reduce the beam spot from approximately 4.5 by 3 centimeter to a 1-centimeter diameter circular spot. A test object that consisted of a 10-centimeter diameter right circular cylinder of polyethylene inserted into a 15 centimeter outside diameter, 10 centimeter inside diameter tube of depleted uranium was radiographed at several different angular orientations. The radiography magnification was set to about 1/20, so the expected position resolution was somewhat less than 1 millimeter. Three holes with diameters of 1.2, 0.6 and 0.3 centimeters were bored parallel to the axis of the polyethylene.

Some theoretical tomographs of the cylindrical test object were calculated using the standard flux for WNR 4FP30R and neutron-total cross sections. Neutrons for energies between 50 and 700 MeV were included in the calculations. A finite WNR source size of 1 centimeter was used, but there was no attempt made to model resolution smearing by nuclear scattering. The calculations are direct geometrical integrations, statistical effects are also not included. These results are shown on the left in figure 2. The image produced from the actual data is displayed on the right. In the tomographic reconstructions shown in figure 2, all three holes are visible.

Because the holes in the polyethylene represent neutron transmission variations of only 1-3%, they would not be easily visible in a reconstruction of the complete object.

To make them visible, the nine views were first averaged and then each individual view was divided by this average prior to linearizing.

The resulting reconstructions are shown in figure 2.

Low-Energy Neutron Detectors

A second objective focuses on developing new techniques for detecting neutrons at and below thermal energies. The long-term goal of this effort is to make available a new technology for large-area, inexpensive position-sensitive (wallpaper) detectors. An immediate goal is to provide detectors in support of current LANSCE experiments.

Neutron detection requires a converter in which the neutron produces a charge signal and a technique to detect the charged signal. At low energies, exothermic neutron absorption reactions, such as $^3He(n,p)^3H$, are used. Because of its large cross section and large-energy release ^3He is the most commonly employed converter for thermal energy neutrons. In some applications, ^6Li or ^{10}B are employed. At thermal energies and below, the cross sections for these reactions scale as 1/v, where v is the neutron velocity. For ^3He the cross section, σ, is 500 barns at 1.8 Ångstroms. The mean free path, λ, is $1/\rho\sigma$ = 42 centimeter/bar/$\sqrt{}$eV and the efficiency, *eff*, is given by: $eff = 1 - \exp(-l/\lambda)$.

Scintillators, solid state detectors, and amplifying gas structures have all been employed as detectors. Of these proportional-chamber detectors are the most common because of ease of construction, ease of operation, and expense. In addition to the ^3He, a higher-density stopping gas is usually needed to limit the range of the charged particle range in order to prevent energy transfer to the detector walls and to limit the size of the interaction so that position resolution requirements can be meet. We built a gas handling system, which allowed us to study different gas mixtures and recover the ^3He. We used this to study various stopping gases.

Ultracold Neutron (UCN) Detectors

We have designed and built UCN detectors for use at LANSCE. These are stable detectors with very good signal-to-noise ratios. The background rates were on the order of 0.02 counts/second. These low backgrounds enabled us to detect UCN at a rate of less than 1 count/second in our first year of running with the rotor source. We have since improved many aspects of the source and are now up to a production rate of 800 counts/second. In addition to wall losses, one needs to worry about upscattering of the UCN before they are detected. We have found that the low scattering cross sections for fluorine and carbon make CF_4 an ideal stopping gas for UCN detectors.

A photograph of our UCN detector is shown in figure 3. The performance of the detector for detecting UCN is shown in figure 4, where a two-dimensional histogram of time *vs.* pulse height is shown. The band of uniform pulse heights with no time correlation is due to UCN. The low velocity of the UCN washes out the 50 millisecond period of the LANSCE spallation source.

Line Readout Detector

Position sensitive area detectors for neutrons are commercially available. Most of these rely on a capacitive-resistive(RC) delay line for encoding the position information. Although this technique is capable of providing good position resolution, ~1% of the delay line length, it is comparatively slow. Typically, several microseconds are required to provide an analog position signal. This long time leads to problems at short times (fast neutrons) because of pileup. It is not unusual for this to lead to a several millisecond long dead time at the leading edge of the neutron pulse. We investigated fast delay line encoding as a solution to this problem. Although this technique has been in use for some time[2] in high nuclear physics, it has not been tried for low energy neutron detectors.

We completed and tested a 5-centimeter by 40-centimeter active area, fast delay-line-readout, two-dimensional imaging detector for cold neutrons and used it in the focal plane of the Bragg spectrometer on the ultracold neutron (UCN) rotor on flight path at LANSCE. The data from this detector helped us to verify that dynamic distortions of the Bragg reflector were not large enough to influence the UCN production rates. The advantage of this detector over more conventional RC-network encoding detectors is that it is much faster and essentially immune to dead time caused by the gamma flash.

^{3}He Ion Chamber

We also designed, built, and used a helium-3-filled ion-chamber detector for monitoring neutron fluxes from LANSCE beam lines. We developed a method for obtaining absolute flux measurements by analyzing the fluctuation levels from the detector.

Large Area Detectors

A final objective targets large-area, inexpensive neutron detectors. We began a development project aimed at designing and constructing inexpensive amplifiers and readout electronics for large-area pad-readout ion-chamber detectors. They should provide a low-cost alternative to the area detectors currently used for neutron work.

The mean free path, λ, for thermal neutron in ^{3}He is about 6 bar-centimeter. This establishes the minimum cost for an area detector.

The cost of the ^3He for a two-λ thick (86% efficient) detector is about \$24000/m^2. High-energy physics has developed the techniques needed for cathode pad readout of multi-wire proportional detectors. It is possible to instrument a pad with a low noise amplifier and readout for about \$4/channel.

For a 1 centimeter-square segmented readout this adds another \$50000/m^2 of cost. It should be possible to produce detectors at a fraction of the cost of current techniques.

Noise levels of several thousand electrons can be achieved for modern pulse amplifiers. Since the charge produced in a neutron interaction in ^3He is about 2.5×10^4 no further amplification is needed. This implies that large area ion-chamber structures with segmented readout can provide an inexpensive alternative to multi-wire chambers as low-energy neutron detectors. The absence of wire planes or micro-etched circuit boards for added gain reduces the mechanical complexity of the detectors and allows more flexibility in their mechanical design. For instance it should be possible to design such a detector to conform to the surface of a sphere.

Publications

None

References

[1] C, L. Morris *et al.,* "An Integrating Image Detector for High Energy Neutron Radiography," the 5th International Conference on Applications of Nuclear Techniques-Neutrons in Research and Industry, Crete, Greece, June 9-15, (1996).

[2] L. G. Atencio, J. F. Amann, R. L. Boudrie, and C. L. Morris, "Delay-Line ReadoutDrift Chambers," *Nucl. Instrum. Methods* **187**, 381 (1981).

Figure Captions:

Figure 1: Radiograph of a drill motor made with a 1.5 millimeter thick copper converter coupled to a single image plate. The neutron source was WNR 4FP30R.

Figure 2: Left: reconstruction from modeled data; Right: reconstruction from the actual data. The pixel size is about 1millimeter /pixel. The data outside of the polyethylene insert are not reliable because of the beam size. All three holes in the polyethylene can be observed in both the model and the data.

Figure 3: Photographs of the UCN detector

Figure 4: Two-dimensional histogram of time on the horizontal axis and pulse height on the vertical axis.

Figure 5: Photographs of the delay-line readout detector.

Figure 6: Two-dimensional histogram of Bragg spectrum from the moving rotor.

Figures

Figure 1

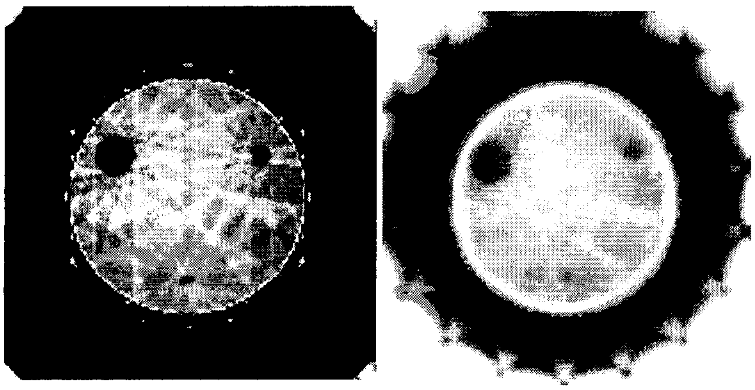

Figure2

Figure 3

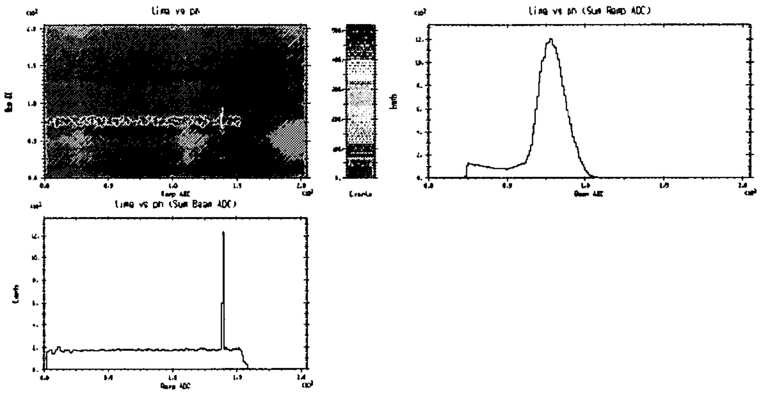

Figure 4

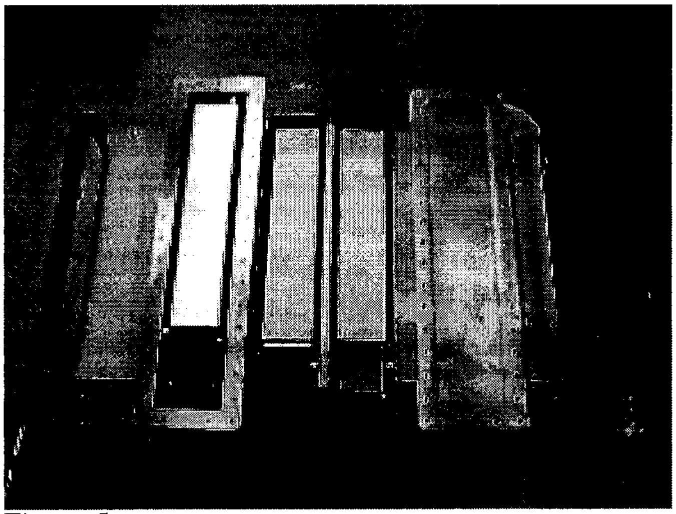

Figure 5

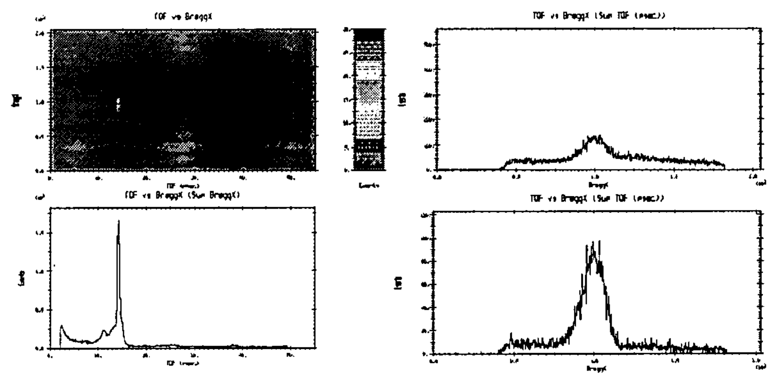

Figure 6

B. Beam Optics and Choppers for Neutron Scattering-Scattering Applications

Background and Research Objectives

The importance and rationale for studies of magnetic materials with reduced dimensionality is that the understanding of many (if not all) the interesting magnetic phenomena in microstructures relies on a detailed knowledge of the magnetic structure. This work reflects areas of research where the bulk material has been extensively studied and is believed to be well understood, but differences in the magnetic properties of materials occur when their length scales are reduced to the nanometer size. In many cases, the implicit assumption is made that the bulk magnetic structure is preserved even in these unusual geometries that approach atomic length scales. This is clearly incorrect. There are very few probes that can give detailed information regarding the magnetic structure at interfaces—neutron scattering is probably the most powerful of them. It is incumbent upon us now to develop neutron scattering techniques suitable for a pulsed-neutron source with which studies of nanostructured magnetic materials can be made.

In 1994, Brockhouse and Shull were honored with the Nobel prize for their contributions to physics in the field of neutron scattering. Much of Shull's work involved determining magnetic crystal structures, i.e. the spin configurations of magnetic lattices. Shull's pioneering work demonstrated the importance of neutron scattering in understanding magnetic phenomena; consequently, neutron scattering is often cited and recognized as one of the most important tools for understanding these phenomena. At the Institut Laue Langevin (Grenoble, France) and other modern reactor sources, where advances in neutron scattering beyond those achieved through gains of intensity, have greatly improved our understanding of magnetism. Specifically, hot and cold neutron diffractometers at reactor sources polarize the neutron beam before the sample and determine its polarization after the sample. By measuring changes in the polarization of a neutron beam before and after the sample, the sensitivity of neutron scattering to weak magnetic spin correlations is greatly increased. Ferromagnetic correlations in the metallic phase of V_5O_9 were identified with the aid of polarization analysis. It is now believed to be the onset of ferromagnetic correlations that are responsible for the metal-to-insulator transition in V_5O_9, rather than the development of antiferromagnetic correlations more typical of a Mott insulator. Today, considerable interest in determining the magnetic lattices of bulk materials requires the detection of subtle correlations near phase transformations, e.g. metal-insulator transitions in V_5O_9 or Ca-doped $LaMnO_3$, or correlations that develop in the presence of very large magnetic fields (e.g. the 30-T pulsed-magnet) or under high pressures. Identification of ferromagnetic correlations will be a task for which polarized neutron scattering is the tool-of-choice for many years to come.

Since Shull's first work, technological advances in sample preparation (e.g. multilayers with well-defined interfaces), characterization and processing (e.g. electron beam lithographically-defined dots showing mesoscopic phenomena) have opened up new areas of physics in which structural length scales can play an important role in determining the magnetic properties of materials (e.g. induced polarization in a non-magnetic material by a magnetic material). Sometimes the magnetic properties of an artificially-structured material can be quite extraordinary. Take for example, the observation of Schuller's group (UCSD) of the magnetization bias of a simple Fe film when deposited onto a thin single crystal FeF_2 film. Under certain field-cooling conditions, the magnetization of the Fe film is reversed with the application of a field on the order of 1kOe. The inability to reverse the magnetization of the ferromagnet (FM) with small magnetic fields involves an interaction between the magnetic spins of the antiferromagnet (AFM) and FM across the AFM-FM interface. Use of so-called exchange coupling is the heart of spin-valve devices in the latest magnetic read-heads. Industry has a huge financial interest in understanding the origin of exchange-coupling, and its wider use in magnetic devices of the future.

Importance to LANL's Science and Technology Base and National R&D Needs

To achieve a detailed understanding of complex materials, future studies will use neutron beams to characterize the exotic magnetic and atomic structures of these materials in combination with never-before-realized conditions of high magnetic field, high pressure and very low temperatures. Studies such as these would ultimately contribute to materials studies pertaining to the Laboratory's core mission through the design of materials relevant to weapons applications. High strength alloys would be an example of such materials.

Scientific Approach and Accomplishments

There are hundreds of other examples in which polarized neutrons produced at reactor sources, where use of polarized neutrons is a big business, have aided our understanding of materials. The scarcity of polarized neutron work using pulsed-spallation sources is due to the lack of adequate know-how, and technology. Presently, polarized neutron scattering at pulsed-neutron sources involves a small number of experiments restricted to the use of polarization attachments on reflectometers. These experiments use at most a few percent of the neutron flux available to the (unpolarized) instrument. To make efficient use of the pulsed-neutron source for polarized neutron work requires: (1) production of purely polarized "white" cold neutron beams with large cross-sectional areas, e.g. 60centimeter^2 (2) control (through flipping) of the beam polarization, and (3) polarization of the neutron beam scattered by the sample covering large solid angles.

These developments can be achieved using existing supermirror technology and should allow us to perform conventional elastic scattering measurements with polarized neutrons second to none in this country or at any pulsed-neutron source world-wide. We can do even better. We can also exploit the pulsed nature of the LANSCE source to study inelastic magnetic scattering (e.g. the separation of elastic scattering from inelastic diffuse scattering arising from fluctuations of magnetic correlations) with statistical flipping of the neutron beam polarization on a microsecond time scale, and to examine changes in magnetic correlations after pulsed-excitations of the sample, e.g. excitations produced by a 30-T pulsed magnet or by a pulsed-laser. These capabilities would be truly novel, and are examples of neutron scattering that could be done at LANSCE and not even conceived of at a reactor source. This project aims to develop a competency in the production and use of polarized neutrons at spallation sources with which we will be able to perform experiments at the forefront of neutron scattering.

This effort resulted in the production of $2m^2$ of polarizing transmission supermirrors. The magnetic properties of these mirrors were characterized with magnetometry and polarized neutron reflectometry. The magnetization of the mirrors were found to be highly anisotropic (a desirable feature) whose hysteresis loops were exceedingly square. Near remanence, the mirrors retained 95% of their saturation magnetization (Fig. 7); thus, these mirrors are expected to polarize neutron beams in near zero-field conditions (also highly desirable). Results from tests (one of 192 such tests are shown in Fig. 8) of the polarization properties with neutrons were promising. Sophisticated analytical techniques widely employed within the Japanese industrial community were used to evaluate and rank-order the quality of nearly 100 mirrors.

Publications

None

References

None

Figure Captions

Figure 7: Magnetometry measurements of a typical mirror fabricated for this project showing the ferromagnetic hysteresis loops along the easy and hard axes. The large remanent magnetization of the mirror for fields applied parallel to the easy axis, is crucial for zero-field neutron beam polarization. For comparison, a measurement is shown taken from a conventional supermirror coating.

Figure 8: The flipping ratio is related to the polarization of the neutron beam. The mirrors fabricated for this project typically produce neutron beam polarization of >95%— more than sufficient for most neutron scattering applications.

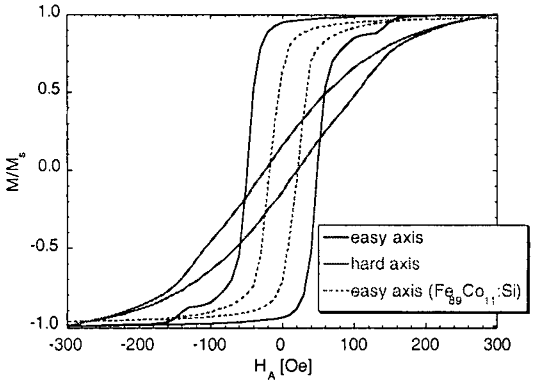

Figure 7

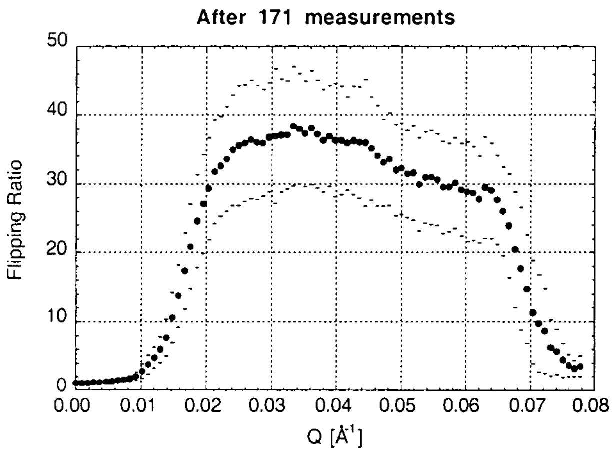

Figure 8

C. Development of Time-Resolved Cold-Neutron Radiography Methods

Background and Research Objectives

Neutron radiography is an attractive technique in non-destructive testing and evaluation due to the strong energy variation of neutron cross section characteristics of nearly all the nuclides. As a result of this strong variation, measurement of the neutron transmission as a function of energy and position can be used to give elemental and spatial information about an object over a broad band of neutron energies. Neutron radiography has been carried out primarily at reactors where a steady state source of neutrons covering a broad energy range is available. Spatial resolutions of a few tens of microns can be obtained readily in such radiographs and resolutions as high as 1 micron has been reported by the Phoenix Memorial Laboratory at the University of Michigan.

The neutron source at LANSCE not only provides a capability to carry out neutron radiography at Los Alamos using thermal and cold neutrons, but because LANSCE is a pulsed source it offers a unique capability to carry out radiography at specific neutron energies over the thermal and cold neutron energy range. Using the Bragg cutoff phenomena of a number of materials, energy specific radiography can be used to identify materials and discriminate among various materials. Such a capability is of interest to the DOE stockpile management and Stockpile Stewardship Program at Los Alamos and other DOE laboratories.

An additional advantage to using the spallation neutron source at the Lujan Center is that the neutron beam has very low gamma contamination. Unlike at a reactor where there is a high gamma flux along with the neutron flux, the neutron beam on FP 11a has almost no gammas. Thus, radiographs using traditional film techniques and not-so-traditional amorphous silicon techniques can be made without the additional complication of unavoidable gamma exposure that is often present in a reactor environment.

We have carried out radiography on test components using three imaging techniques, time-gated imaging, an amorphous silicon detector, and conventional x-ray film. Materials discrimination using time-gated imaging was demonstrated for the first time at LANSCE and we demonstrated that relatively high resolution imaging could be obtained using an amorphous silicon detector and conventional x-ray film. We radiographed a Sandia National Laborator y-supplied test sample of a cracked fire-set case to determine if such cracks could be imaged with neutron radiography and we obtained radiographs clearly showing the crack with a resolution estimated to be between 5 and 10 microns. In a collaboration with the Phoenix Laboratory, we radiographed two jet engine nozzles to determine if coking could be observed in the nozzles. This test demonstrated that higher resolution would be needed in the beam line to observe the small amounts of coking in jet engine nozzles for which such detection is needed.

Scientific Approach and Accomplishments

Time-Gated Cold Neutron Radiography

Neutron radiography with cold neutrons using time-gating is a technique that was first demonstrated at LANSCE. This technique is of interest because of an important behavior of crystalline materials at cold neutron energies. Below an energy of a few meV (the exact energy depends on the material), there is an abrupt drop in the scattering cross section when the wavelength reaches twice the largest d-spacing of the material. The energy level where this abrupt drop occurs is referred to as the Bragg cutoff. This behavior is not exploited in a reactor environment because the steady state nature of the neutron source is not favorable to separating neutrons of different energies. However, a pulsed neutron source, such as is available at LANSCE, can employ time-of-flight to obtain radiographs at specific neutron energies (or in a narrow range of specific neutron energies). By recording image data at different times during a neutron pulse, radiographs can be made at neutron energies of interest, for example, just above and just below the Bragg Cut-off of a given material. Consider a sample or device made of components of various materials. A radiograph taken at an energy above the Bragg cutoff of all the components in the device would show the entire device. However, choosing an energy below the Bragg cutoff of some materials and above the Bragg cutoff of others produces a radiograph having the "below the Bragg cut-off" components much less absorbing than the remaining components. Thus, it is possible by judiciously choosing the neutron energy at which a radiograph in made to separate components and materials in a sample or device. With this technique, it is possible to obtain multiple radiographs emphasizing some components or constituents and de-emphasizing others, without modifications to the object. These component images can likely be separated through signal processing. In addition, imaging in three dimensions can be obtained using tomographic image reconstruction techniques.

This phenomenon was demonstrated on a flight path at the Lujan Center. A silvered lithium zinc sulfide scintillator (Bicron 704) was used as a neutron to light converter and the image on the scintillator was relayed by a mirror to a gated intensified camera. The demonstration was carried out using two materials that have a well defined Bragg cutoff, beryllium, which has a Bragg cutoff at approximately 6 meV, and carbon, which has a cutoff at approximately 1.9 meV. A 25-millimeter thick beryllium block was obtained into which a one-half by 20 threaded hole was cut (one-half inch diameter and 20 threads per inch). A one-half by 20 carbon screw was inserted into the hole. Radiographs were made above, between, and below the two Bragg cutoffs. The results of the radiography are shown in Fig. 9. Fig. 9a shows a radiograph taken at approximately 7.5 meV, which is above the Bragg cutoffs beryllium and carbon. Above the Bragg cutoffs both the beryllium and carbon show up relatively dark in the radiograph because the scattering cross section is high. The portion of the carbon bolt inside the beryllium cannot be observed. Fig. 9b shows a radiograph taken at approximately 2.9 meV, which is between the Bragg cutoffs of the two materials, and the beryllium has become much lighter because the scattering cross section has significantly decreased while the carbon bolt remains relatively dark. That portion of the carbon inside the beryllium has now become visible. Fig. 9c shows a radiograph taken at approximately 1.5 meV, which is below the Bragg cutoff of both materials, and both materials have become light in the radiograph and that portion of the carbon in the beryllium is no longer visible.

Although this phenomenon is material dependent and is not exhibited for all materials, we believe there are enough materials, such as carbon and iron, for which an abrupt change is exhibited that the approach can be exploited in programs of interest.

Radiography using an Amorphous Silicon Detector

Use of an amorphous silicon detector was also demonstrated at the Lujan Center. The advantage of the amorphous silicon detector is that, unlike a CCD silicon detector, it can be placed directly in the neutron beam path with effectively no damage if the beam is not left on the detector for long periods of time. Thus, there is no need to relay the image using optics and a good quality image (tens of microns) can be obtained relatively quickly (within a few seconds). Unfortunately, the amorphous silicon detector cannot be gated and, thus, cannot be used for gated imaging. Figure 10 shows an example of an image we obtained with a Reticon amorphous silicon detector.

Radiographs with X-ray Film

The highest quality and resolution radiographs we have obtained have been with x-ray film. A thin gadolinium foil is placed next to the film and produces x-rays proportional to the local neutron flux. The x-rays expose the film. Figure 11 shows a radiograph of a cracked fire-set sample provided by Sandia. We estimate the resolution of this radiograph to be between 5 and 10 microns. As with the amorphous silicon detector, gated imaging cannot be obtained with the film technique.

Possible Applications

The use of cold and thermal neutron radiography appears to have applications in the DOE stockpile maintenance and Stockpile Stewardship Program (weapons stockpile surveillance related programs) and in industry. Six potential applications have been identified in the weapons stockpile surveillance programs and one potential industrial application has been identified.

Weapons Stockpile Surveillance Related Applications

The first application involves determining the water content in desiccant. Oak Ridge National Laboratory has provided a mock device for testing this concept, which we plan to radiograph during the next run cycle.

A second application is the determination of electrical breakdown paths in failed PZT generators that are used in some weapons related applications. Sandia fabricates these generators and when failures occur it is difficult to diagnose the cause. The PZT crystal is encapsulated and the breakdown path in within the encapsulant; physically opening the device disrupts the breakdown path and prevents an effective cause analysis. Sandia has asked if we could obtain a radiograph of the breakdown track in a failed device to assist with determining cause of failure. A third application is the study of gas flow in a gas handling apparatus. Because of the pulsed beam at LANSCE we may be able to study the dynamics of the gas flow in the device. A fourth application is the determination of voids and defects in detonators. A fifth application involves determining the uniformity of materials in a fire-set case for Sandia. The case is fabricated from epoxy reinforced with borated glass fibers. It is approximately 5 millimeter thick and 45 centimeter in diameter. We have demonstrated that a crack in the material can be observed with good resolution and we are optimistic that the composite noise ratio can also be used to observe inhomogeneities in the material make up. The sixth application, which is more uncertain than those previous, involves the radiography of bulk material assemblies to identify possible anomalies and defects in the assembled materials. Because the bulk assemblies have relatively high mass, we are somewhat skeptical that effective radiography can be carried out at the Lujan Center and we plan to first study this application through simulation.

Industrial Applications

We currently plan to assess two industrial applications. One is to determine the extent of solid hydrocarbon deposits in jet engine fuel nozzles. The condition of hydrocarbon deposits in fuel nozzles is referred to as coking and this particular application appears to be well suited for cold or thermal neutron radiography because it involves imaging a light material within a heavy material. X-ray radiography cannot be used for this application. Neutron radiography appears to be well suited for this application, however, our initial attempts to radiograph nozzles demonstrated that improvements are needed in the resolution of the beam line. We are considering possible approaches to making such improvements. A second application is determining nonuniformities and inhomogeneities in a sheet of polymer material that has recently been developed by an industrial firm. Although only two industrial application has been identified, we believe many more exist and we plan to aggressively identify and test additional applications of interest to industry.

In summary, potential applications that we have identified at the present time are listed below.

Weapons Related Applications (Stockpile Stewardship Program)

- Water content in desiccant (Mock Assembly from ORNL)
- PZT Electrical Generators Breakdown Track
- Dynamic Gas Flow in Gas Assemblies
- Detonator Defects
- Fire-set Case Inhomogeneities
- Bulk Assembly Anomalies and Defects
    - Moisture Content
    - Cracks
    - Movement
    - Industrial Related
- Extent of Coking in Jet Engine Nozzles
- Nonuniformities and inhomogeneities in Sheet Material

Publications

None

References

None

Figure Captions

Figure 9 Demonstration of cold neutron radiography using time-of-flight and gated imaging to obtain radiographs at specific neutron energies. These images demonstrate materials discrimination using the Bragg cutoff phenomenon. The images are a series of radiographs of a carbon bolt threaded into a beryllium block. Image (A) is a radiograph taken at approximately 7.5 meV, which is above the Bragg cutoffs of both beryllium (6 meV) and carbon (2 meV) and shows both the beryllium and carbon relatively dark. Image (B) is a radiograph taken at approximately 2.9 meV, which is between the Bragg cutoffs of beryllium and carbon; the beryllium has become lighter due to the reduction in scattering cross-section across the Bragg cutoff and the carbon bolt inside the beryllium has become visible. Image (C) is a radiograph taken at a neutron energy of approximately 1.5 meV, which is below the Bragg cutoff of both beryllium and carbon and both the beryllium and carbon have become lightened. Note that if any denser material had been obscured by the beryllium and carbon materials it could be seen in Image C. Fig. 1a Neutron Energy: 7.5 meV Above Cutoff of Be (6 meV) Above Cutoff of C (2 meV) Both Be and C Dark; Fig. 1b: Neutron Energy: 2.9 meV Below Cutoff of Be Above Cutoff of C, Be Light; C Dark; Fig. 1c: Neutron Energy: 1.5 meV Below Cutoff of both Be and C, Both Be and C Light

Figure 10: Neutron Radiograph taken with a Reticon amorphous silicon detector. The sample is a 25-millimeter thick beryllium block with threaded holes (20 threads per inch) into which are screwed a nylon screw (left) and a brass fitting (right). An aluminum nut has been fully screwed onto the nylon screw and can be seen abutting the screw head. Also seen in the image is a nylon 0-ring inside the brass fitting. Such an o-ring would not be visible in an x-ray radiography. The resolution of this neutron radiograph is approximately 150 microns. The dark vertical lines in the image are columns of defective pixels in the detector.

Figure 11: This image is an example of the highest resolution radiography that has been achieved on the LANSCE CNR facility. The image is a radiography of a cracked fire-set case sample provided by Sandia. The radiograph is an experiment to determine if such a crack could be imaged by neutron radiography. The crack is well defined in the radiograph with a resolution estimated to be in the neighborhood of 10 microns. The radiograph was obtained with x-ray film; a thin foil of gadolinium was placed next to the film to serve as a neutron to x-ray converter

Figures

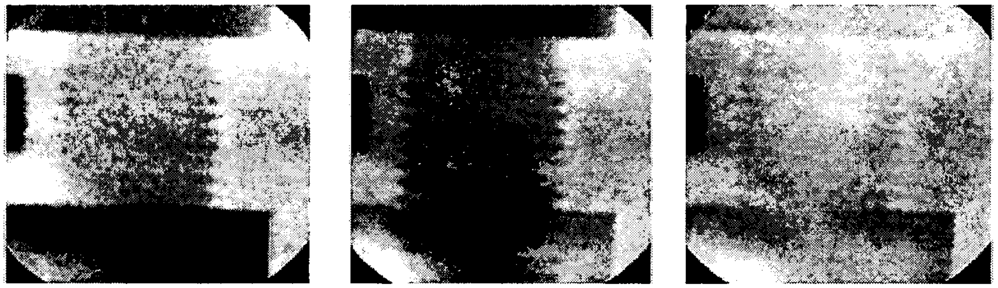

Figure 9

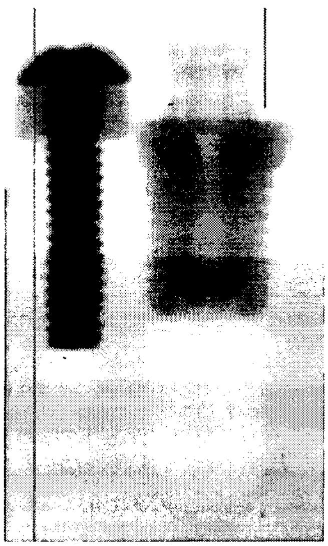

Figure 10

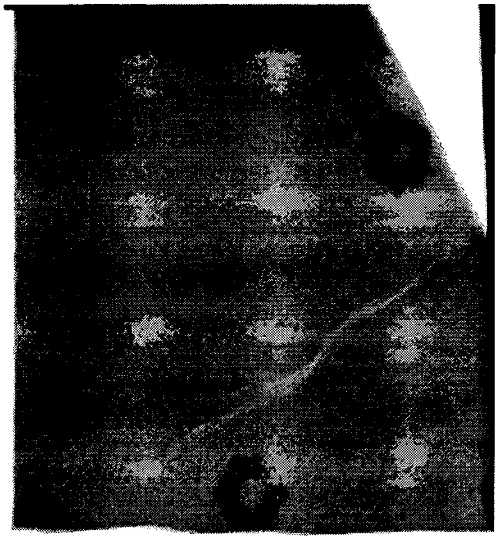
Figure 11

D. Development of Monte-Carlo Simulation Tools for Neutron Instrument Design

Background and Research Objectives

Unlike x-ray generators, neutron sources have inherently low brightness, and care must be exerted in the design of neutron scattering instruments and their coupling to the source to ensure optimal use of the beam. Our research focussed on the development of a relatively general, versatile Monte Carlo tool for the computer simulation of neutron optics and neutron scattering instruments that allows a user to produce computer models of an instrument and study its performance quantitatively. NISP –the Neutron Instrument Simulation Package- is not based on ray tracing; it implements a wide range of neutron optics models to describe neutron transport (including gravity) and scattering the optical elements making up the instrument. The program is freely available to anyone at http://strider.lansce.lanl.gov/NISP/Welcome.html

The purpose behind the development of the Neutron Instrument Simulation Package (NISP) is to provide the community of neutron scatterers with a general, versatile tool similar to the SHADOW code for optical design of photon scattering instrumentation. NISP is a family of Monte Carlo codes to assist in the design and analysis of neutron optical components and neutron scattering instruments.

Importance to LANL's Science and Technology Base and National R&D Needs

The computer code supports the development of new neutron scattering instruments at the Manuel Lujan, Jr. Neutron Scattering Center at LANL. It is also useful to optimize the performance of existing instruments, to analyze experimental results, to teach neutron scattering techniques, and to test new ideas in the fields of neutron scattering and neutron optics. NISP complements widely used neutron transport codes developed at LANL (such as MCNP) by extending these codes to the optical regime. NISP overcomes the limitations of a ray-tracing approach in designing new instruments and allows the user to match an instrument with its moderator so as to maximize neutron use. In view of the cost and difficulty in producing intense neutron beam, instrument optimization is absolutely essential. With no computer code possessing the depth, generality, and flexibility of NISP, the research described below filled a gap not only within the Laboratory, but also in the neutron scattering community at large.

Scientific Approach and Accomplishments

NISP has three main components, all of which were developed extensively during the course of our research.

MCLIB: a library of Fortran subroutines that deal with elementary tasks such a geometry representation, neutron transport, and contains all the models for optical elements. Associated with this library is a set of source files representing more than 25 different types of moderators and a set of scattering kernels for sample simulation, as well as various data files with physical constants for materials.

MC_RUN: a Monte Carlo engine that runs the Monte Carlo simulation itself and produces a series of output file with detector output and general information about the outcome of the simulation. MC_RUN takes care of neutron propagation in the instrument and tallies neutrons at all relevant places in the instrument.

MC_Web: A WWW-based application that allows the user to set up the instrument geometry interactively without having to learn any of the data structures of MCLIB. MC_Web is based entirely on object-oriented concepts within the framework of the well-known GemStone package.

<u>*New MCLIB developments include:*</u>

- new algorithms for Fermi choppers, benders, Soller collimators (straight and tapered), material cross section, various sample scattering kernels, curved detectors, detector encoding in spherical and cylindrical coordinates, monochromator crystals (flat and curved), tapered guides, multilayers, radial collimators, current loops, solenoids, etc...
- new moderator source files for LANSCE, IPNS, ISIS, HFBR, and SNS

MC_RUN work focussed largely on code optimization to speed up simulation, as well as on the development of a formalism to allow for polarized neutron transport. No other code currently has the latter capability. In particular, we developed a numerical algorithm for the fast resolution of the Bloch equations for spin precession. The algorithm is quite general and encompasses adiabatic and non-adiabatic spin transport.

The capabilities of MC_Web were greatly extended:

- extensive revision of the graphical features user interface;
- addition of on-line features to download the code and its accompanying documentation;
- development of on-line help message to guide the user in the selection of device parameters;
- 3-D instrument geometry visualization capabilities based on the virtual reality language VRML (Figure 1);
- calculator to facilitate unit conversions;
- test features for debugging new device algorithms;

- various features allowing users to exchange, copy, delete, and modify instrument definitions.

A User's Manual and a Tutorial were written and made freely available to users.

See_MC-Data, a GUI was developed for the Windows operating system to allow users to visualize and manipulate the histograms produced by MC_RUN.

Benchmarking of the code was also a priority, particularly in FY2000. We modeled a variety of instruments at pulsed and reactor sources and compared the results of calculations with NISP to whatever experimental data was available. For instance, we compared the count rate and energy resolution of the IRIS spectrometer with NISP calculation. The results agreed to better than 5%. We also conducted extensive comparisons of the effect of the PHAROS Fermi chopper on the neutron beam with NISP predictions. The H-8 triple-axis spectrometer at the HFBR was mocked up in great detail. The results of NISP calculations were within 20% of vanadium and gold foil activation data taken more then 15 years ago. Comparisons of the (calculated) NISP source term for the LANSCE liquid hydrogen moderator with measured features of the actual moderator were performed. Benchmarking of the new spin precession algorithm was based on comparisons with analytical models, as well as experimental data provided by F. Tasset at the ILL. Algorithms for crystal and multilayers reflectivity were validated by comparisons with analytical models.

The NISP team was also involved in an international attempt to standardize the format of subroutines for neutron optics in an effort to minimize duplication of efforts among various laboratories and allow these groups to use algorithms developed elsewhere.

Our effort has resulted in several publications in refereed journals and conference proceedings, as well as in three invited presentations at international conferences and workshops(SPIE Conference on "Radiation Sources and Radiation Interactions," Denver, July 1999; Neutron Optics in the Next Millennium, Institut Laue-Langevin, Grenoble, November 1999; SNS Workshop on "Monte Carlo Codes for Neutron Scattering Instrument Design," Oak Ridge, January 2000).

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3. L.L.Daemen, P.A.Seeger, T.G.Thelliez, and R.P.Hjelm, SPIE Conference on "Radiation Sources and Radiation Interactions", E.J.Morton, Ed., Proceedings of SPIE, Vol.**3771**, p.80 (1999).
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7. P.A. Seeger and L.L. Daemen, "Numerical Solution of Bloch's Equations for Spin Precession," to appear in Nuclear Instruments and Methods, September 2000 issue.
8. P.A. Seeger, L.L. Daemen, T.G. Thelliez, and R.P. Hjelm, Physica **B283**, 433 (2000).

References:
None

Figure Caption:
Figure 12: A 3D view of the HIPPO powder diffractometer to be built in the year 2000 at the Manual Lujan Jr. Neutron Scattering Center at Los Alamos National Laboratory as part of an ongoing upgrade project.

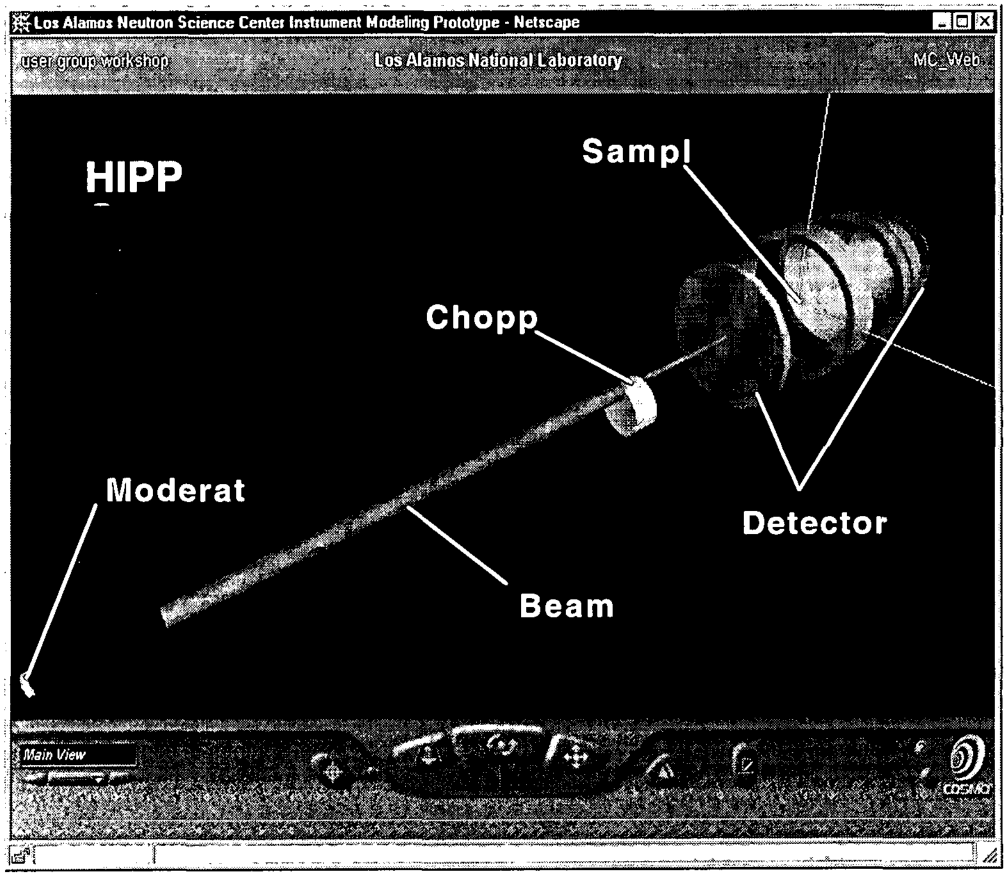

Figure 12